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INVESTIGATION OF THE COLLISION OF METASTABLE ATOMS OF He(2^3S) WITH MOLECULES OF N_2 AND O_2.

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ABSTRACT

Presented are the results of a study of the differential scattering of He atoms in the (1^4S) and (2^3S) states in oxygen and nitrogen. The experimental data are treated using an additive model of the interaction potential, and the parameters of the potential are found. It is observed that the scattering of metastable atoms of He(2^3S) in oxygen and nitrogen is less well described by the given potential model than that of He atoms in their lowest energy state. The results obtained are discussed. /2

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A laboratory study of the collision of metastable atoms of He(2^3S) with molecules of atmospheric gases is quite interesting in connection with understanding the kinetic processes in the upper atmospheres of earth and the planets, and in plasma-chemistry. One particularly interesting problem, not yet solved, is the generation of superheated He atoms capable of overcoming the earth's gravitational field and providing the observed particle flux escaping from the atmosphere.

In this paper, using the technique of scattering fast beams at small angles [1], we investigate the elastic scattering of He atoms in the state (1^1S) and in the metastable (2^3S) states on molecules of N_2 and O_2 in their lowest energy states. A detailed description of the apparatus used has been given in reference [2], and hence we shall limit consideration to a short description of its main units. The set-up consists of a Nirov-type ion source, a magnetic mass analyzer, which separates out ions of the desired mass, a recharging chamber to obtain neutral particles from ions, a deflecting condenser in which the ions not recharged are ejected from the main beam, a scattering chamber with electromagnetic valve (used to admit the scattered gas alternately into the scattering chamber or into an evacuated enclosure), and a detector, located on the axis of the unscattered beam for measuring the integral cross sections and moved in a circle around the center of the scattering chamber when measuring the angular distributions. /3

The recharging chamber is an oven with controlled wall-temperature and, thus, alkali metal vapor was used, together with gas targets, for the recharging. According to [3], with $E = 600$ ev, the recharging of He+ ions in Na vapor is described by the ratio of the total recharging cross sections in the (2^3S) and (2^1S) states, equal to 13.5, and thus to form a neutral beam it is desirable to populate the metastable 2^3S-level.

An electron multiplier was used as the particle detector; it yielded a sharp increase in the sensitivity and a considerable improvement in the resolution of recording the scattered particles. Recording was in terms of discrete counts.

The differential scattering of He atoms in oxygen and nitrogen was studied using beams with an energy of 600 ev, in the range of angles of deflection of the detector $\alpha = 2 \times 10^{-3}$ to 3×10^{-2} rad. For future reference we established the relationship between the scattering cross section and the measuring detector (in the angular position α) by the particle flux $I(\alpha)$. In the case of spherical scattering symmetry the differential scattering cross section in the element of solid angle is related to the sighting distance b by the expression $\sigma(\theta) = (b/\sin\theta)|db/d\theta|$ [4]. This expression can also be used for an anisotropic interaction with a potential $V(r, \Omega)$ with a fixed orientation $\Omega \equiv \{\varphi, \chi\}$ (by angle of deflection we mean, as before, the angle between the asymptotes of the perturbed and unperturbed trajectories). Then the particle flux in the detector $I(\alpha)$ is

$$I(\alpha) = \frac{B}{4\pi}\int\limits_{(\Omega)} d\Omega \int\limits_{(\theta)} \sigma(\theta, \Omega) f_\alpha(\theta) \sin\theta \, d\theta = \frac{B}{4\pi} \iint\limits_{(\Omega)(b)} b f_\alpha(\theta(b, \Omega)) \, db \, d\Omega. \quad (1)$$

Here B is a constant including the known parameters of /4
the experiment [5], $\theta = \theta(b, \Omega)$ is the deflection angle with an orientation angle Ω, $f_\alpha(\theta)$ is a function of the equipment describing the recording effectiveness of the detector of the position α of a particle deflected by angle θ. Integration over $\Omega \equiv \{\varphi, \chi\}$ yields the average over the orientation angles φ, χ.

For spherically symmetrical potentials the average over the angles vanishes, and, assuming a monotonic trend of $\sigma(\theta)$ expression (1) can be inverted -- i.e. from the expression for $I(\alpha)$ we obtain the expression for $\sigma(\theta)$.

The systems studied here relate to a class of complicated multi-electron systems for which there exists no reliable theoretical data regarding the potential energy surface.

In the attempt to interpret the experimental data in terms of the potential we of necessity were faced with the selection of a potential model.

We used an additive model of the potential surface corresponding to pair repulsion between all atoms of the interacting particles $V = \sum_i V(r_i)$ (here r_i is the distance between the i-th atom of the target and a beam atom).

In the classical approximation, which is quite valid for the systems in question within the deflection angle range being considered, and with known $f_\alpha(\theta)$, the calculation of the differential cross section (and hence the particle flux in the detector $I(\alpha)$ using (1)) reduces to finding the deflection function $\theta(b, \varphi, \chi)$. The angles φ and χ establish the orientation of the molecule relative to a fixed coordinate system tied to

the plane xy, perpendicular to the relative velocity vector $\vec{v}$ (Fig. 1). Calculation of $\theta(b, \varphi, \chi)$ for a given set of b, φ and χ turns out to be quite simple for small-angle scattering ($\theta \ll 1$; $V/E \ll 1$), which is the case in this experiment. Then, /5
using the known results of [6], the calculation is reduced to finding the modulus of the lateral momentum vector (i.e. in the xy-plane), equal to the sum (additive potential) of the momenta over all pairs of atoms of the interacting particles. The deflection angle is then determined from the expression

$$\theta E = \left\{\left(\sum_i x_i \mathcal{P}_i\right)^2 + \left(\sum_i y_i \mathcal{P}_i\right)^2\right\}^{1/2}.$$

Here

$$\mathcal{P}_i = \int_{b_i}^{\infty} \frac{dV}{dr} \frac{dr}{\sqrt{r^2 - b^2}}, \quad b_i = (x_i^2 + y_i^2)^{1/2},$$

x_i and y_i are the projections of the interatomic distances in the coordinate plane.

The calculation of the flux $I(\alpha)$, for various positions α, was accomplished with the Monte Carlo method on the BESM-4 computer, and $\sim 10^4$ trajectories, differing in initial values of b, φ and χ, were used to obtain the necessary statistical accuracy of $\sim 3\%$. The interatomic repulsion for the selected potential surface model was approximated with an exponential function with parameters A, β, whose numerical values were found from the condition of superposition of the measured and computed function $I(\alpha)$.

For systems including helium atoms in the lowest energy level, the interaction (repulsion)shows up clearly, and the interpretation of the measurements on the basis of the potential considered is quite well-defined.

The solid lines in Figs. 2 and 3 denote the experimental functions (the bars represent the scatter of the measurements) for the $He(1^1S)$-N_2, O_2 system. The points on these diagrams represent computations using the values of the parameters given in the table. /6

It is pertinent to note, as contrasted with the integral cross sections used earlier [6], that agreement between measured and computed functions $I(\alpha)$ can be realized with different combinations of β and A. To eliminate this ambiguity together

System	β[$Å^{-1}$]	A (ev)	$\bar{\beta}$[$Å^{-1}$]	$\bar{A}$(ev)
$He - N_2$	3.0	80	2.83	154
$He - O_2$	3.1	75	2.95	160
$He^* - N_2$	2.8	90	2.7	187
$He^* - O_2$	2.7	75	2.54	141

with the computation of $I(\alpha)$, the integral cross section was computed, with an energy of 600 ev, using formula (1) and the appropriate equipment function $f_0(\theta)$ [5]. The combination of $I_{calc}(\alpha)$ and $Q_{calc}(E)$ with the measured values permits the selection of a unique combination of A and β; these values are given in the table. Also given in the table are the parameters $\bar{A}$ and $\bar{\beta}$ of the exponential approximation of the additive-type potential, averaged over the orientations (i.e. spherically symmetrical).

The data given illustrate the effectiveness of the method for solving the inverse problem, using data on the angular distribution of the scattered particles. The $He-N_2$ system was investigated independently by measuring the integral cross sections in Amdur's paper [7]. The interaction energies obtained with the spherical-symmetry approximation ($V = 74/r$ ev, $1.79 \leq r = 2.3$Å can be compared with our results for the spherically-symmetrical averaged potential. The comparison indicates good /7
agreement of the potential interaction energies in the interval 1.8-2.3Å.

Let us now consider the findings of studies of the interactions of metastable atoms of He* in the 2^3S state with N_2 and O_2 molecules. The solid lines in Figs. 4 and 5 represent the experimental functions $I(\alpha)$ for the scattering of the metastable atoms on N_2 and O_2. The points on these curves are computed values using (1) for the interaction potential (additive type) for exponential repulsion with the parameter values given in the table.

It should be remarked that the scattering of metastable atoms of He* on both N_2 and O_2 is somewhat more poorly described by this potential than is the scattering of He in the lowest energy level. This could signify that the adopted interaction scheme (pure repulsion) is inadequate; thus the interaction energies obtained for the parameters in the table can be made more precise.

It is well-known that the scattering of metastable atoms He (2^3S) can be accompanied by Penning ionization of partners. Also we should not rule out the possibility of ionization resulting from the interaction of adjacent terms of the perturbed and ionized systems; thus, for the He-O_2 and He-O_2^+ systems (and, correspondingly, for molecules and vibrationally-excited ($\vartheta = 4$) ions N_2^+) the asymptotic energies essentially coincide. Both these factors can significantly perturb the scattering pattern from that anticipated for elastic interaction. In both cases the inclusion of the perturbing channel takes place at large separations, but in the first case transitions are possible for any point on the path, while in the second case transitions should be localized near the point of intersection of the terms. The weak dependence on the energy of the quenching cross sec- /8
tion of He* (2^3S) in nitrogen noted in reference [8] gives a basis for considering that the Penning process is the mechanism preferred over quenching for the energies studied. In this way, the observed scattering pattern can obviously be obtained by taking into account the possibility of a "jump-over" from a term lying in the continuous spectrum to a term corresponding to the system He-N_2^+ (O_2^+).

Corroboration of these hypothesis may be forthcoming at a future date.

To summarize these remarks we can conclude that collisions of this type cannot be a source of fast helium atoms -- otherwise we would observe a non-monotonic trend of the function $I(\alpha)$, and in seeking an alternative collision mechanism for generating fast particles, the system He^+-O_2, N_2 should be similarly examined. /9

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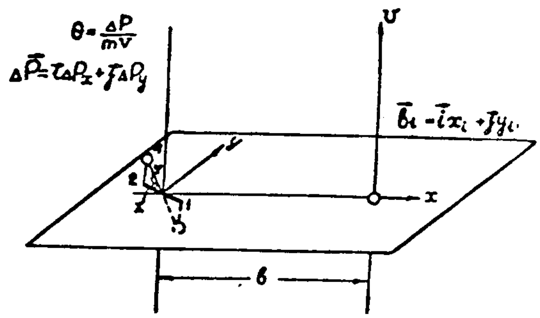

Fig. 1. System of coordinates used to describe the scattering of atoms and molecules.

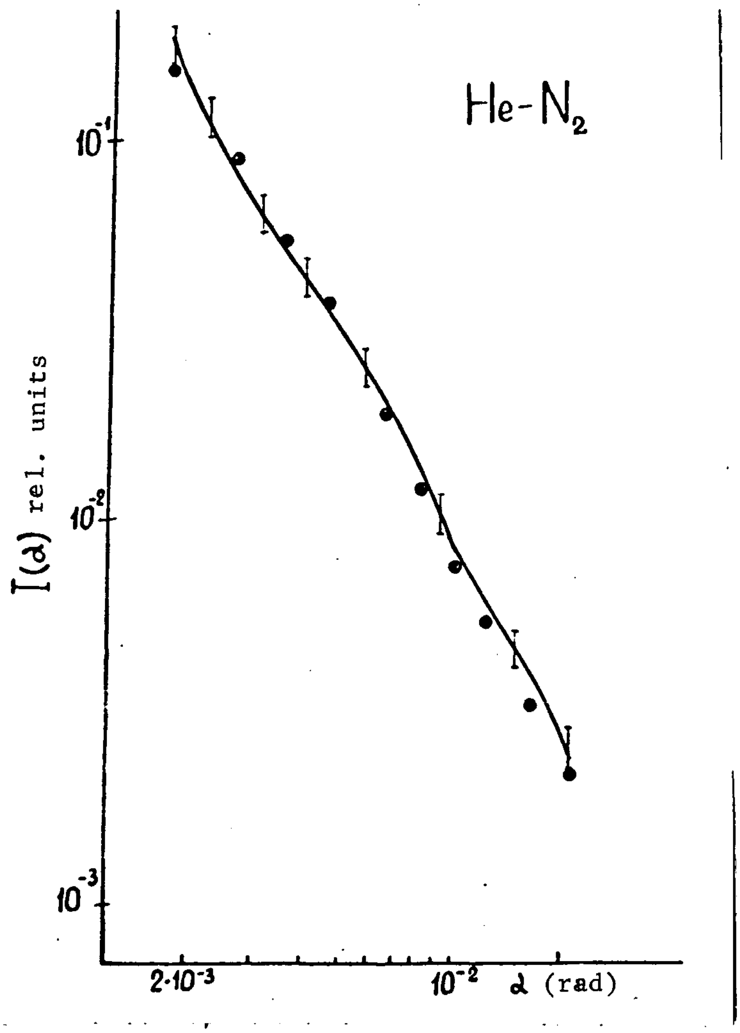

Fig. 2. Angular distribution of I(α) for the scattering of He(1^1S) atoms in nitrogen (the solid line denotes the experimental relationship, the bars the scatter of the measurements, the points the computational results).

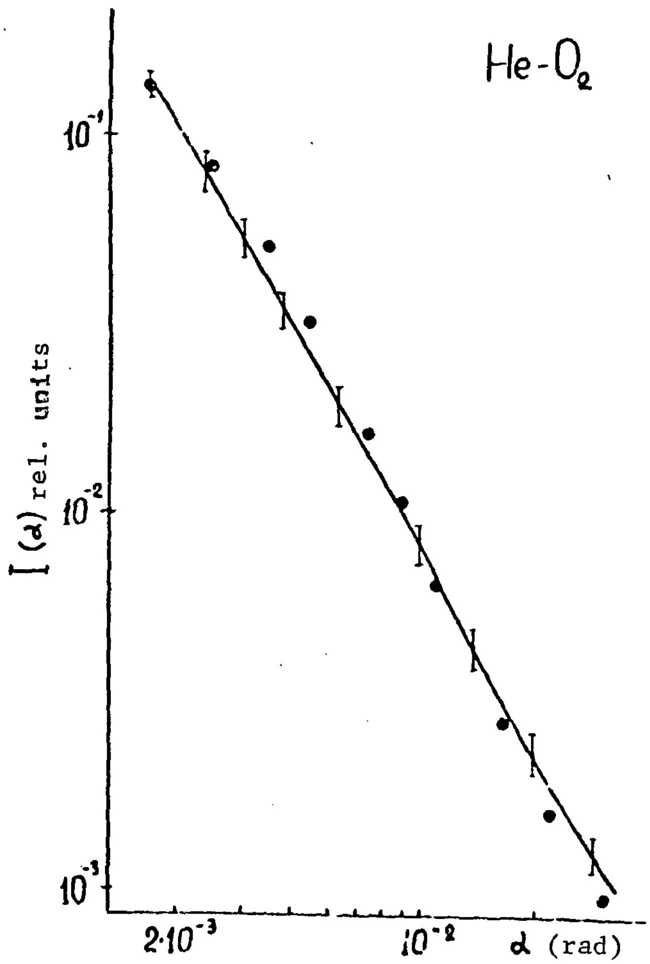

Fig. 3. Angular distribution of I(α) for the scattering of He(1^1S) atoms in oxygen. (The solid line represents the experimental relationship, the bars the scatter of the measurements, the points the computed results.)

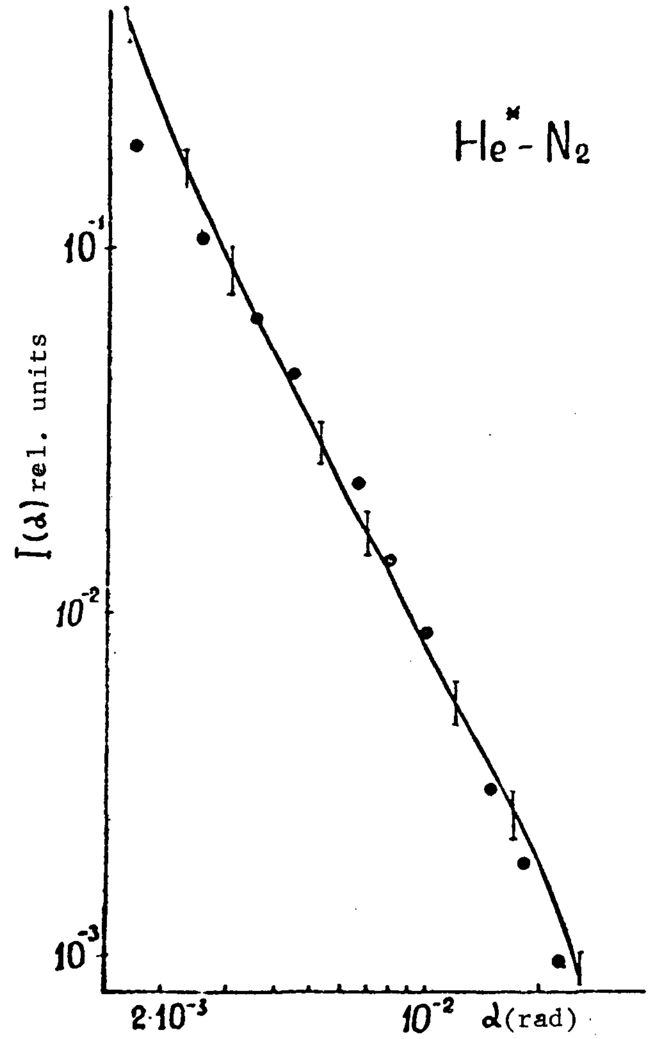

Fig. 4. Angular distribution of $I(\alpha)$ for the scattering of He(2^3S) atoms in nitrogen (the solid line represents the experiment, the bars the scatter of the measurements, the points the calculated results).

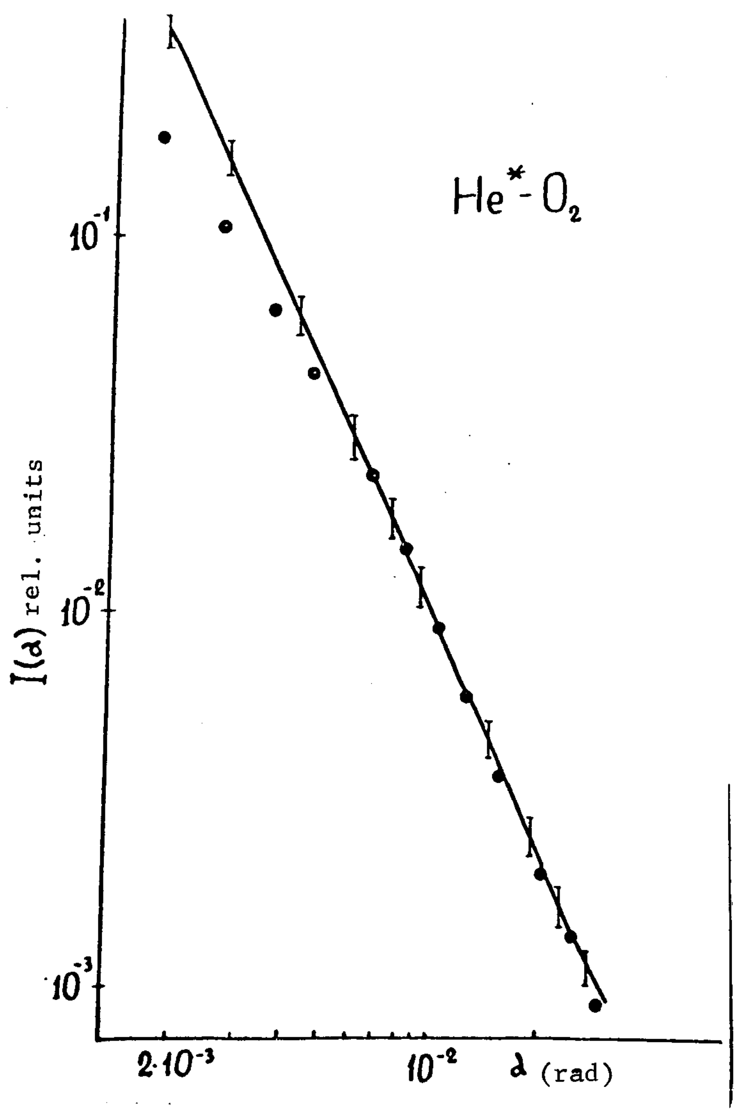

Fig. 5. Angular distribution of I(α) for the scattering of He(2^3S) atoms in oxygen (the solid line denotes the experiment, the bars the scatter of the measurements, the points the calculated results).

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